Ground state of the spin-$\frac{1}{2}$ Heisenberg antiferromagnet on a two-dimensional square-hexagonal-dodecagonal lattice

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Up to now, the existence of the the magnetic Néel Long Range Order (NLRO) in nearest neighbor, spin-$\frac{1}{2}$ antiferromagnetic (AF) lattice systems has been examined for seven, from the eleven existing, two-dimensional, uniform lattices. Plaquettes forming these uniform (Archimedean) lattices (e.g. square, triangular, kagomé) are different regular polygons. An investigation of the NLRO in the ground state of AF spin systems on the seventh uniform (bipartite) lattice consisting of squares, hexagons and dodecagons is presented. The NLRO is shown to occur in this system. A simple conjecture concerning the existence of the NLRO in the ground state of antiferromagnetic, spin-$\frac{1}{2}$ systems on two dimensional, Archimedean lattices, is formulated.

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I. INTRODUCTION

Despite of a great progress, stimulated originally by the discovery of high-T_c superconductivity, made in last years in the understanding of the nature of the ground state of quantum Heisenberg antiferromagnets for low values of spin variables on two-dimensional lattices, the problem is far from being solved. The basic question, if there exists the Néel Long Range Order (NLRO) in the ground state of an antiferromagnetic spin-$\frac{1}{2}$ system on a given lattice is still not completely answered. In fact, a subtle interplay between quantum effects and lattice effects, rather difficult to deal with, may lead to nontrivial properties of the ground state. Restrict now the attention to the most simple case of spin system with equal, antiferromagnetic, nearest neighbor interactions:

$$H = \sum_{<i,j>} \vec{S}_i \cdot \vec{S}_j. \tag{1.1}$$

The natural way to represent this kind of spin system is to put the spins onto vortices of a so-called uniform (Archimedean) lattice and to assign the antiferromagnetic spin-spin interactions along the lines connecting the nearest spins. *Uniform* means that all polygons of the smallest area built from nearest neighbor interactions (plaquettes) are regular, and consequently, each lattice site has the same local environment. For example, in the case of a kagomé lattice there exist two kinds of such polygons: triangles and hexagons. Up to now, the problem of the eventual existence of the NLRO in a spin-$\frac{1}{2}$ system residing on a uniform lattice has been investigated for seven uniform lattices only. Let us summarize the results of those investigations. First, take into account *unfrustrated* lattices. In the case of square[1], honeycomb[2] and CaVO[3] lattices there exist a well grounded opinion that the ground state is Néel-like ordered. For *frustrated* lattices, however, the situation is more complicated. There exist three sublattice magnetic order in spin-$\frac{1}{2}$ system on the triangular lattice[4–7] and probably does not exist in the case of kagomé lattice[8]. For zig-zag-ladder lattice[9] it seems to exist an incommensurate spiral order. The most complicated situation is for the model examined by Shastry and Sutherland[10] and more recently by Albrecht and Mila[11] which corresponds to a Heisenberg antiferromagnet on an uniform lattice for $J_1 = J_2$ (notation taken from Ref. [11]). In that case spin wave theory gives a disordered ground state, whereas Schwinger-boson mean field theory predicts NLRO. However, for $J_2/J_1 \approx 1.1$ NLRO becomes unstable and gives way to spiral order[11].

We formulate now the simple conjecture which seems to apply to the problem of the NLRO in the ground state of spin-$\frac{1}{2}$ systems with nearest neighbor interactions on uniform lattices. At first, however, let us classify all investigated so far uniform lattices according to the number of edges of polygons of the smallest area bound by the nearest neighbor interactions. There exist three possible cases: *i)* only even polygons (i.e., with even number of edges) are present, e.g., square lattice - squares, honeycomb lattice - hexagons, CaVO lattice[3] - squares and octagons. Call those lattices the even ones. *ii)* only odd polygons are present, triangular lattice - triangles. This is the only one odd lattice and *iii)* even and odd polygons are present, e.g., kagomé lattice - hexagons and triangles, zig-zag-ladder lattice[9] and Shastry

- Sutherland lattice[10] - squares and triangles. Those are even-odd lattices. The above classification allows one to formulate the following conjecture: the antiferromagnetic spin-$\frac{1}{2}$ system on an even-odd lattice has no NLRO in its ground state. If the lattice is even *or* odd - the ground state is Néel-like ordered.

The aim of this paper is to report an additional example which does support this conjecture. This example concerns the spin-$\frac{1}{2}$ system located on the last possible, yet not investigated, even Square - Hexagonal - Dodecagonal (SHD) lattice, see Fig. 1. Note that there exist only four even, one odd, and six even-odd uniform (Archimedean) lattices.

II. METHOD

To answer the question about the NLRO in the ground state of the spin system on the *bipartite* lattice from Fig. 1 a variational approach developed by Huse and Elser[12] and improved later to restore the S^x, S^y symmetry by Carneiro, Kong and Swendsen[13] was applied. It was also shown that within this method one can obtain reliable results for both magnetically Néel ordered and disordered systems[12,14]. Let us remind the basic points of this method. At the beginning, the variational wave function is expanded into the complete set of Ising states $|\alpha\rangle$ in the subspace of total $S^z = 0$:

$$|\Psi\rangle = \sum_\alpha \exp(\frac{1}{2}\tilde{H}) |\alpha\rangle, \tag{2.1}$$

and the operator $\tilde{H}$, diagonal in that base is defined as

$$\tilde{H} = 2\pi i(\sum_{i \in B} \frac{1}{2} - S_i^z) + \sum_{i,j} K(r_{ij}) S_i^z S_j^z. \tag{2.2}$$

The first term produces a proper sign (phase) for a given state $|\alpha\rangle$ (the first sum runs over spins belonging to the B sublattice) whereas the second one, taking into account in a variational way the long-range correlations in the spin system, gives the value of the amplitude for that state. The second sum runs over all possible pairs of spins. The next step of this method is to find a minimum of the ground state energy $\langle\Psi|H|\Psi\rangle/\langle\Psi|\Psi\rangle$ with respect to parameters $K(r_{ij})$ and, subsequently, to calculate for those $K(r_{ij})$ the expectation values of the operators which characterize the LRO in the ground state of a given spin system. In the case of small clusters this can be accomplished by taking into account the whole subspace of Ising states, in the case of larger ones - within a Monte-Carlo approach[12,13]. Finally, those values are extrapolated to the thermodynamic limit.

Actually, two expectation values of such operators were calculated: the squared sublattice magnetization and, which is new within this approach, the spin gap, i.e., $E_1 - E_0$, where E_0 and E_1 stand for the ground state energy (sector $S^z = 0$) and the energy with one flipped spin (sector $S^z = 1$), respectively.

How to choose the variational parameters $K(r_{ij})$ in Eq. (3) for the bipartite SHD lattice? Several choices of the parameter space were tested in variational calculations done for spin systems on finite clusters of other bipartite lattices: for 18 spins on the linear chain and on the honeycomb lattice, for 16 spins on the CaVO lattice and for 12 spins on the SHD lattice. The whole $S^z = 0$ basis in expansion (2) was taken into account. The minimal value of the variance of the ground state energy has been obtained in all cases in three parameter space: (K_{AA}, K_{AB}, σ). It means that $K(r_{ij}) = K_{AA}/r^\sigma$ when spins at the distance r_{ij} belong to the same sublattice, $K(r_{ij}) = K_{AB}/r^\sigma$ otherwise, and r_{ij} is the Manhattan metric (the shortest path over bonds), instead of the commonly used Euclidean one. Henceforth all expectation values of operators are calculated for the latter choice of the variational parameters.

III. RESULTS

To estimate the quality of this approach to the problem, the ground-state energy, the squared magnetization, the correlation function for the highest distance in the cluster and the spin gap were calculated by the direct diagonalization and, in addition, the variational approach described above. The results for some clusters on different bipartite lattices are collected and compared in Table I. Notice that for all clusters considered in this paper periodic boundary conditions were used. In the variational approach all the base functions of the $S^z = 0$ subspace were taken into account. From Table I one can see that this variational method overestimates a little bit the tendency towards LRO - the variational values m^2 and the correlations are bigger than the exact ones and the variational values of the spin gap are smaller than the exact ones.

Now, let us take into account larger clusters. The variational results for 48-, 108-, and 192-spin clusters are collected in the Table II and the finite size analysis is presented in Figs. 2 - 5. It has also been checked that the energy minimum

for the lattice of 108 spins is attained for values of the variational parameters $K_{AA} = -2.77$, $K_{AB} = -2.85$, and $\sigma = 1.17$, different but very slightly from those for 48 spins, so it was decided to keep them unchanged in the calculations for 192-spin cluster.

One can assume that the leading term of the finite-size correction of the ground state energy per bond E resulting from the cutoff of the long-wavelength magnons which are linear in k, is, like in the case of other translationally invariant systems, $N^{-3/2}$. The data from Table II can be fitted to this dependence and hence the energy per bond, E_∞ in the thermodynamic limit is obtained: $E(N) = E_\infty + aN^{-3/2}$ with $E_\infty = -0.3605$ and $a = -0.8200$. This dependence is shown in Fig. 2. Using in the fitting only the data for 48, 108 and 192 spins one obtains $E_\infty = -0.3607$, and practically the same value of E_∞ gives fitting to the formula $E(N) = E_\infty + a'N^{-3/2} + bN^{-2}$.

In Fig. 3. the order parameter squared as a function of the system size $N^{-1/2}$ is depicted. The square of order parameter should scale as $N^{-1/2}$, therefore, for small N, corrections of higher orders may be important. Thus we decided to take into account only the data for $N =$ 48, 108 and 192 spins in the extrapolation. This leads to the following form for the square of sublattice magnetization as a function of N: $m^2(N) = m_\infty^2 + cN^{-1/2}$ with $m_\infty^2 = 0.1007$ and $c = 0.5058$. One can conclude that the long-range magnetic order persists in the ground state of this spin system.

Finally, an additional argument, supporting the existence of the NLRO order, is presented in Fig. 4 which shows the extrapolation of the spin gap to the thermodynamic limit according the relation $\Delta(N) = \Delta_\infty + dN^{-1}$ with $\Delta_\infty = -0.0260$ and $d = 6.514$. Note that the value of d is consistent with the leading-order spin wave result[15] for the finite-lattice energy gap: $\Delta(N) = 2zN^{-1} + \ldots$, where z is the number of nearest neighbors. Keeping in mind the tendency of the variational method to the underestimation of the spin gap one can regard the ground state as being gapless.

IV. SUMMARY

In this paper, the first investigation of the ground state of the Heisenberg spin-$\frac{1}{2}$ system on square-hexagonal-dodecagonal lattice is presented. The calculated valus of m_∞^2 and Δ_∞ seem to be an evidence for the existence of two-sublattice Néel long-range magnetic order in this system. This result can also be regarded as an argument supporting a very simple conjecture concerning the existence of the magnetic NLRO in the ground state of the Heisenberg antiferromagnets on uniform lattices, however further studies, especially for even-odd lattices, supporting (or not) this conjecture are required.

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FIG. 1.   SHD (Square-Hexagonal-Dodecagonal) lattice. The fourth uniform, even, bipartite lattice. Sublattices are marked by circles and squares. Spins residing on A-sublattice interact only with its nearest neighbors from B-sublattice. The 48-spin cluster used in calculations is also marked. Other clusters have the same shape.

FIG. 2.   Energy per bond for the spin system on the SHD lattice as a function of $N^{-3/2}$.

FIG. 3.   Plot of the m^2 as a function of $N^{-1/2}$. Squares - values obtained by applying the variational method. Straight line - fit to the squares. Sizes of squares are comparable to the error bars.

FIG. 4.   Plot of the spin-gap $\Delta = E_1 - E_0$ vs $1/N$. Errors result from adding the errors for E_0 and E_1.

TABLE I. Comparison between exact and variational results for finite clusters for different bipartite lattices.   All the variational results were obtained in three parameter space K_{AA}, K_{AB}, σ.

		linear chain 18-spin cluster	honeycomb lattice 18-spin cluster	CaVO lattice 16-spin cluster	SHD lattice 12-spin cluster
Ground state	exact	-0.4457	-0.3740	-0.3800	-0.3850
energy, per bond	variational	-0.4450	-0.3698	-0.3733	-0.3803
m^2	exact	0.1851	0.2481	0.2504	0.2913
	variational	0.1859	0.2509	0.2616	0.2979
correlation for largest	exact	0.0859	0.1655	0.1468	0.1924
distance in cluster	variational	0.0752	0.1714	0.1724	0.2032
gap	exact	0.241	0.394	0.446	0.568
	variational	0.241	0.323	0.378	0.519

TABLE II. The ground state energy, the squared sublattice magnetization, the energy of the first excitation E_1 and the spin gap for some clusters on SHD lattice. In a case of 12 spin cluster the values were obtained in the whole $S^z = 0$ sector, for bigger clusters the Monte-Carlo method was applied. Statistical errors, in parantheses, are the last digit.

N	$E_0/bond$	m^2	E_1	$E_1 - E_0$
12	-0.3803	0.2979	-6.3285	0.519
48	-0.3628(4)	0.1743(8)	-26.014±0.019	0.107±0.038
108	-0.3614(2)	0.1476(6)	-58.506±0.034	0.042±0.060
192	-0.3609(2)	0.1384(5)	-103.948±0.019	0.003±0.080